

Meteorology

Numerical simulation of the temperature distribution of coffee stored in cooled and natural environments

Simulação numérica da distribuição de temperatura de café armazenado em ambientes resfriados e naturais

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ABSTRACT

The storage of agricultural products is of great importance in maintaining product quality between harvest and commercialization. The use of numerical and computational techniques, such as the finite element method (FEM) and computational fluid dynamics (CFD), allows the analysis and simulation of systems that involve heat transfer, as is the case of grain storage. A computational model based on these techniques that satisfactorily represents a real system was used to test and to analyze decision alternatives without the need for real experimentation. In this study, we sought to study the behavior of the temperature of a mass of stored mocha coffee beans by using computational techniques, as requested by the private sector. The coffee was stored for 6 months in two types of environments: a cooled environment between 15 and 18 °C by using an air temperature control equipment used for artificial cooling and a natural environment. A computational model was developed to simulate the heat transfer process for both types of storage. In the comparison of the temperature distribution during storage from simulation results and for experimental results, an overall mean relative error of 2.34% was obtained for coffee stored in a natural environment, and that of 5.74% was obtained for coffee stored in a cooled environment.

Keywords: Computational fluid dynamics; Cooled storage; Coffee

RESUMO

O armazenamento de produtos agrícolas é de grande importância para manter a qualidade do produto entre a colheita e a comercialização. A utilização de técnicas numéricas e computacionais, como o método dos elementos finitos (FEM) e a fluidodinâmica computacional (CFD), permite a análise esimulaçãode sistemas que envolvem transferência de calor, como é o caso do armazenamento de grãos. Um modelo computacional baseado nessas técnicas que representa satisfatoriamente um sistema real foi utilizado para testar e analisar decisões alternativas sem a necessidade de experimentação real. Neste trabalho, buscou-se estudar o comportamento da temperatura de uma massa de grãos de café mocha armazenados por meio de técnicas computacionais, conforme solicitado pelo setor privado. O café foi armazenado por 6 meses em dois tipos de ambientes: ambiente refrigerado entre 15 e 18 °C por meio de equipamento de controle de temperatura do ar utilizado para resfriamento artificial e ambiente natural. Um modelo computacional foi desenvolvido para simular o processo de transferência de calor para ambos os tipos de armazenamento. Na comparação da distribuição de temperatura durante o armazenamento de resultados de simulação e de resultados experimentais, um erro relativo médio global de 2,34% foi obtido para o café armazenado em ambiente natural e de 5,74% foi obtido para o café armazenado em ambiente refrigerado.

Keywords: Dinâmica de fluidos computacional; Armazenamento refrigerado; Café

1 INTRODUCTION

Coffee is an agricultural product whose price is strongly influenced by its quality (BORÉM *et al.*, 2019). The factors that compromise quality include the grain chemical composition, postharvest processes (such as storage), roasting, grinding, and beverage preparation. Obtaining competitive prices for the product is possible only with the preservation of coffee quality during storage (BORÉM *et al.*, 2008).

A stored grain mass is subjected to the action of physical, chemical, and biological variables, which together lead to the formation of gradients of temperature, humidity, and gas within the grain mass. The existence of these gradients causes a process of heat and mass transfer within the ecosystem (ANDRADE *et al.*, 2004).

Because temperature is one of the main factors that affects the quality of grain storage, the use of artificial cooling technology has been increasing. This technique consists of cooling the silos or storage sites by means of cooled air blown into their interior, and the system remains in operation until the grain mass reaches desired temperature levels. The objective is to preserve the quality of the products for a

longer time and to reduce their deterioration since the reduction of their temperature decreases the speed of their biochemical and metabolic reactions (PARAGINSKI *et al.*, 2015).

The following systems can be used to cool storage environments that must be hermetically isolated: vacuum cooling systems, where cooling is achieved by the rapid evaporation of the product water; systems with cold water, where the product is immersed in ice water; and forced ventilation systems, the main method used for cooling agricultural products, where cooled external air is injected directly into the storage environment (GROSS; WANG; SALTVEIT, 2016).

Computational models are used for heat transfer analyses in diverse applications, such as in the study of the temperature distribution in furnaces (GARCÍA *et al.*, 2019), the simulation of heat and water transfer during corn drying (OSTANEK; ILELEJI, 2019), and the efficiency of grain dryers (ROMÁN; MBUGE; HENSEL, 2019). A computational model for the numerical simulation of a real situation allows us to propose improvements, to optimize, and to test alternatives to predict which is the best without the need to perform physical experiments (PENG *et al.*, 2017).

This study aimed to simulate the heat transfer process during storage under different conditions and compared the results of the simulation with those observed experimentally. The demand for the project came from the private sector, from a company that stores commodity and specialty coffees, with the need to study new storage techniques that could be used and implemented in its structure.

2 MATERIAL AND METHODS

The methodology used to carry out the project was divided into an experimental methodology and a mathematical and computational methodology, as shown below.

The study was conducted at the Laboratory of Agricultural Product Processing (LPPA, for its abbreviation in Portuguese) of the Federal University of Lavras (UFLA) and at the company LIV in the city of Varginha- MG, Brazil. The municipality has an

average altitude of 980 m. The climate is classified as Cwb (tropical highland climate) in the Köppen-Geiger climate classification.

The coffee used was made available by Nucoffee and was composed of many types of commercial mocha beans, so it may contain different varieties. The product was stored in the company's warehouse (LIV), and the physical and thermal properties were determined and the sensory analysis was performed in the laboratory (UFLA).

The coffee was stored in jute sacks for 6 months - between November 2019 and May 2020 - in a warehouse in the city of Varginha in the conventional way (in the natural environment) and in the conventional way in a cooled environment (15 to 18 °C).

Each of the two piles contained 7 vertical stacks of 10 bags each, totaling 70 bags per pile, with 140 bags in total (one pile in a natural environment and one pile in a cooled environment).

The bags of coffee stored in a cooled environment were isolated inside a polyethylene wrap (Cocoon Lite 005, GrainPro) that minimizes gas and water exchange with the external environment.

Note that the product used to isolate the beans is not intended for the thermal insulation of the stored product, and this information was considered during the set-up of the experiment and in the possible results. The polyethylene wrap was used due to the availability of the product offered by the company, the practicality of using it for storage of sacks, and the ease of adapting it for cooled storage (with inlets and outlets of cooled air in the system, for example) and to scientifically ascertain its efficacy for cool storage.

Figure 1 shows an open cocoon, with the pile inside, and a closed cocoon.

The cocoon model used (Lite 005) had dimensions of 3 m in length, 1.6 m in width, and 1.5 m in height. Although there are two cocoons in Figure 2, only the cocoon on the right was used for cool storage.

A grains and seeds cooler from the company Cool Seed was used to maintain a low temperature inside the cocoon, which allowed the injection of cooled air into the cocoon where the coffee was stored. The equipment was not a commercial model but was built for use in tests and experiments, as in this study.

The cooled air was directed to the cocoon through a pipe positioned at the rear of the cocoon. The static pressure inside the pipe was 100 mmca. Figure 2 shows how the distribution of cool air to the cocoon in the warehouse was achieved.

Figure 1 – Open and closed cocoon for storage of sacked coffee



Source: Author (2020)

Figure 2 – Distribution of cool air from the equipment to the cocoons



Source: Author (2020)

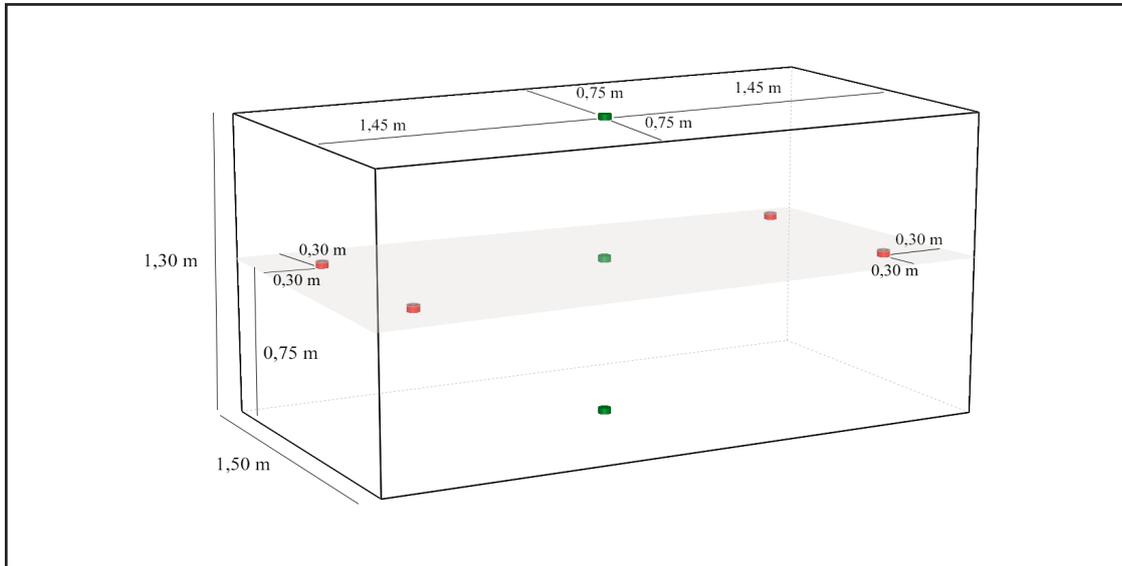
The air-cooling equipment was configured to turn cooling on when the grain mass reached 18 °C and to turn cooling off when it reached 15 °C to keep the temperature within the desired range. The control was performed by the equipment panel, which indicates the current grain mass temperature, the temperature of the air being injected into the pile, and the external ambient temperature.

The temperature inside the piles was monitored throughout the storage period. This monitoring was performed by 22 identical sensors positioned inside and outside the piles, in which 15 sensors were used for the pile in a cooled environment and 7 sensors were used for the pile in the natural environment. Different numbers of sensors were used because the changes in temperature in the cooled environment were greater due to the difference between the temperature of the cocoon environment and the temperature of the outside environment, while the temperature of the pile in the natural environment stabilized with the external environment and did not change significantly.

At the end of the storage period, temperature readings of the sensors were compared to the temperature data obtained by the process simulation, which validated the model as a faithful representation of the real system. The position of each sensor in the piles, identified by a number on its side, was recorded to facilitate comparison with the same position in the simulation.

The sensors for data collection in the coffee pile stored in a cooled environment were positioned at different heights in the vertical stacks. Figure 3 shows a perspective view with all sensors positioned inside the pile and their position. Each point with the same color has the same distance from the side edges and may vary only in height inside the pile.

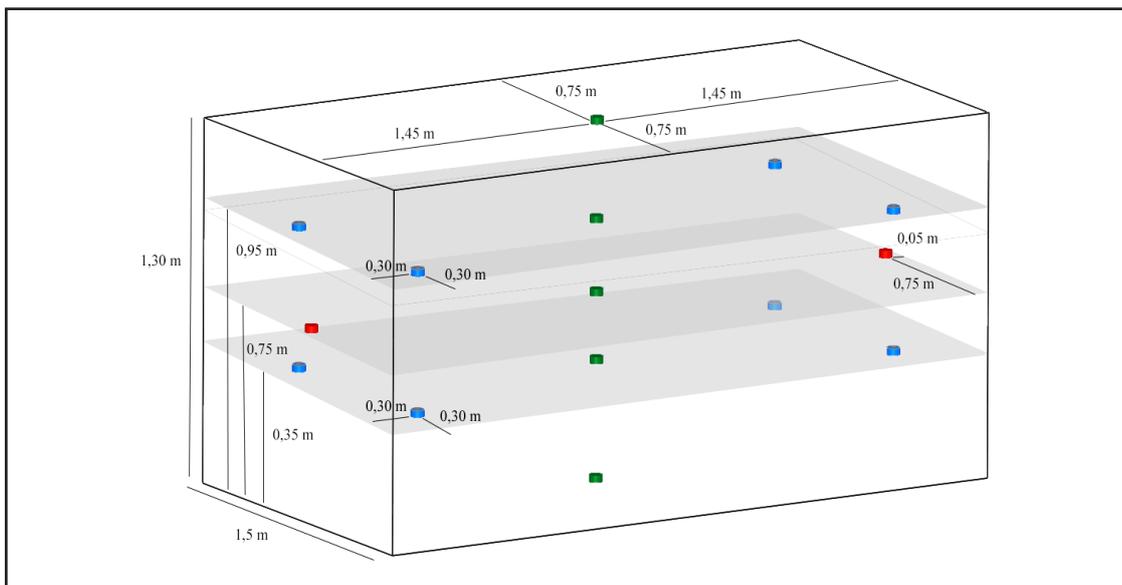
Figure 3 – Perspective view of the 15 collection points inside the pile in a cooled environment and their positions



Source: Author (2020)

Similarly, Figure 4 shows the positioning of the collection points in the coffee pile stored in a natural environment.

Figure 4 – Perspective view of the 7 collection points inside the pile in a natural environment and their positions



Source: Author (2020)

The simulation of the behavior of the storage systems was performed with the finite element analysis software ANSYS Workbench version 20.1 (student), which uses the computational fluid dynamics (CFD) method with models obtained by the finite element method (FEM) to obtain the behavior of systems involving heat transfer.

Two systems were simulated: one in a cooled environment, where the coffee pile is surrounded by a cocoon with the entry of cooled air, and another coffee pile in a natural environment without any type of cooling and with only the coffee pile.

After the numerical simulation, the temperature distribution results were compared to the experimentally obtained results to validate the developed model and to evaluate its reliability in the representation of a real storage system.

In the case of storage with cooling, the three-dimensional modeling of the geometry of the stored coffee bag pile and of the cocoon that surrounds it was performed in SOLIDWORKS software version 2017. The geometry was then exported to ANSYS Meshing version 20.1 (student), a software internal to the ANSYS Workbench, which was used for the choice and application of a mesh to the geometry by subdividing the solid into finite elements.

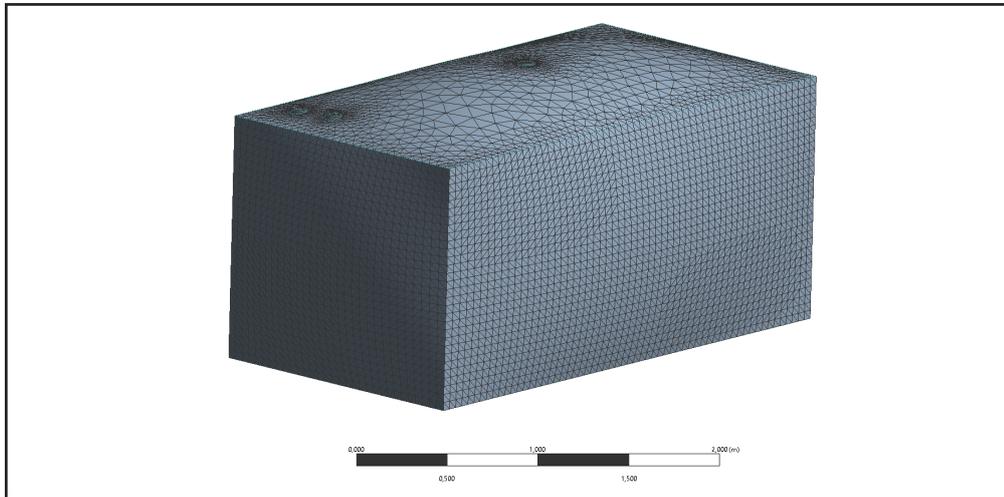
The coffee stack was 1.5 m wide, 2.9 m long, and 1.3 m high. The cocoon was 1.6 m wide, 3.0 m long and 1.5 m high. It contained 2 parallel inlets of cooled air of 0.15 m diameter each and close to the ground level, and 3 air outlets of 0.1 m diameter, one of which was in the center of the upper part and two of which were on the side opposite to the air inlets.

Figure 5 illustrates the composition of the storage system in a cooled environment with the cocoon, which involved the coffee pile, the air inlets, and the air outlets.

It is noteworthy that the storage system in a natural environment consisted only of a coffee pile, with no cocoon wrapping.

The geometry of the storage system in a cooled environment, which consisted of the coffee pile surrounded by the cocoon, was a tetrahedral mesh with 75,453 nodes and 122,170 elements. Figure 6 shows the mesh used for simulation.

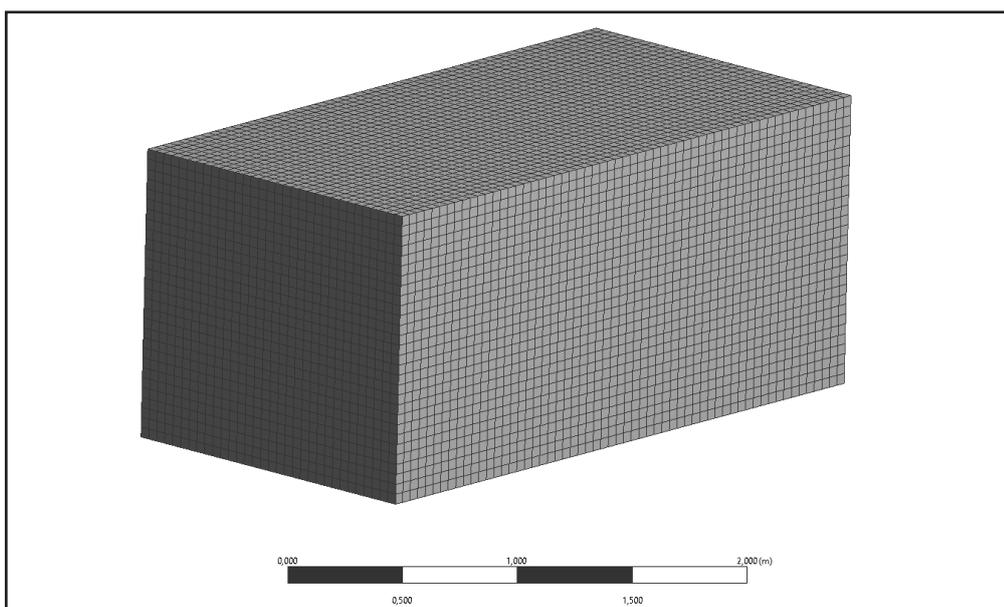
Figure 5 – Mesh applied to the geometry of the cocoon surrounding the coffee pile in the cool storage



Source: Author (2020)

Figure 6 below shows the mesh applied only to the geometry of the coffee pile used for storage in a natural environment. The mesh used in this case was of the hexahedral type and had 49,383 nodes and 45,240 elements.

Figure 6 – Mesh applied to the geometry of the stored coffee pile



Source: Author (2020)

The model assumes the following working hypotheses: transient state (dynamic system in time) and three-dimensional and isothermal flow. As boundary conditions, nonslip conditions were considered for boundaries with solid surfaces.

The equation of conservation of momentum is given by Equation 1.

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{t}}) + \rho \vec{g} \quad (1)$$

where ρ is the density (kg.m^{-3}); p is the static pressure (Pa); $\bar{\bar{t}}$ is the stress tensor (Pa); and \vec{g} is the gravitational force (ms^{-2}).

For the energy dissipation, we have Equation 2.

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} 2\mu_t E_{ij} E_{ij} - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (2)$$

where u_i is the velocity component in the corresponding direction (m.s^{-1}); E_{ij} is the strain rate component (dimensionless); and μ_t is the turbulent viscosity ($\text{m}^2.\text{s}$), in which $\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$; and we have the following constants: $C_\mu = 0.09$; $\sigma_k = 1$; $\sigma_\varepsilon = 1.30$; $C_{1\varepsilon} = 1.44$; $C_{2\varepsilon} = 1.92$.

The energy that governs the model is given by Equation 3.

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot (k_{eff} \nabla T) + S_h \quad (3)$$

where E is the energy (J); T is the temperature ($^\circ\text{C}$); k_{eff} is the effective thermal conductivity ($\text{Wm}^{-1}.\text{C}^{-1}$); and S_h is the heat source term (Wm^{-3}).

The computer used for the numerical simulations had a Ryzen 5 3600 processor operating at 4.2 GHz, 16 GB 2666 MHz RAM, Windows 10 64-bit operating system, version 2004.

The software used for the simulation of the storage systems was ANSYS Fluent version 20.1 (student), a software internal to the ANSYS Workbench. It uses the geometry and mesh previously chosen to represent the physical system.

A total of 12 parallel processes were used for the simulations. The $k-\epsilon$ model was used to predict the turbulence (*standard $k-\epsilon$*). In the simulation of storage in a cooled environment, air enters the system through the two inlets at a speed of 13.0 ms^{-1} , as measured by an anemometer in the real system, and at a temperature of $11.8 \text{ }^\circ\text{C}$, as measured by a thermocouple.

During storage in a real cooled environment, the cooling system turned off a few times when its sensor reached a certain temperature. To more closely simulate the actual operation environment, the time points when the cooling system was turned off and turned on were defined, and they were manually entered in the simulation. For this, a user-defined function was used ("*udf*": *user-defined function*) that maintained the air inlet speed at 13.0 ms^{-1} while the cooling system was on, zeroed the air inlet speed (0 ms^{-1}) when the cooling system was off, and then returned the air inlet speed to 13 ms^{-1} as soon as the cooling system restarted operation.

For boundary conditions, the values obtained by a sensor located outside the system, which obtained data at the same frequency as the internal sensors (every 1800 seconds), were used for the temperature outside the cocoon. In the case of storage in a natural environment, these external temperature values were used for the walls of the coffee pile.

To use these temperature data, which vary every 1800 seconds, an *udf* was used that returns the external temperature for each period to the model. A user-defined functions was used in the simulation model.

The initial temperature of the cooled storage system was defined as $26.4 \text{ }^\circ\text{C}$, which is the mean of the first temperature reading of all sensors at the beginning of storage. For natural storage, the initial temperature of the coffee pile was defined as $27.5 \text{ }^\circ\text{C}$ by using the same criterion.

The physical and thermal properties obtained by the analyses of the initial samples were used for the coffee pile in both storage systems, the remaining volume inside the cocoon (cooled storage) was considered air, and the standard properties for air of the software were used.

In total, 8,516 steps were simulated for each system, with an interval of 1800 seconds (0.5 hours) between them, totaling 15,328,800 seconds or approximately 177 days of storage.

Table 1 shows a summary of the information for the thermo physical properties obtained experimentally (thermal conductivity through the infinite cylinder and specific heat capacity through the mixtures method) and used for the coffee and the input data considered by the model in the simulations.

Table 1 – Thermophysical properties used for coffee and input data for the model

Properties and input data	Value used
Bulk density (kg.m ⁻³)	678.07
Specific heat capacity (kJ.kg ⁻¹ .°C ⁻¹)	1.405
Thermal conductivity (W.m ⁻¹ .°C ⁻¹)	0.111
Initial temperature (cooled environment) (°C)	26.4
Initial temperature (natural environment) (°C)	27.5
Inlet air velocity (m.s ⁻¹)	13.0
Inlet air temperature (°C)	11.8

Source: Author (2020)

To evaluate the quality of the models in representing the real systems, the mean relative error was determined for each temperature collection point for each system (cooled and natural environments), which can be obtained using Equation 4.

$$P = \frac{100}{n} \cdot \sum \frac{|Y - \hat{Y}|}{Y} \quad (4)$$

Where P is the mean relative error (%); n is the number of observations; Y is the experimental value observed at a given point; and \hat{Y} is the value obtained by the model at the same point.

The overall mean of these errors was then calculated for each storage system.

3 RESULTS AND DISCUSSION

For the simulation of each system (cooled and natural environments), the overall mean relative errors were obtained. The results are shown in Table 2.

Table 2 – Overall mean relative errors obtained for each storage system

Storage system	Overall mean relative errors (%)
Cooled Environment	5.74
Natural Environment	2.34

Source: Author (2020)

Overall mean relative errors of 5.74% and 2.34% were observed for the simulations of storage in a cooled environment and in a natural environment, respectively. The higher error value for the cooled environment is higher than that of the natural environment because of the greater complexity of the system as a whole. According to (MOHAPATRA; RAO, 2005), deviations of up to 10% between the actual values and the values obtained from the curve estimated by the model are considered satisfactory and indicate that the model can be used to represent the real situation.

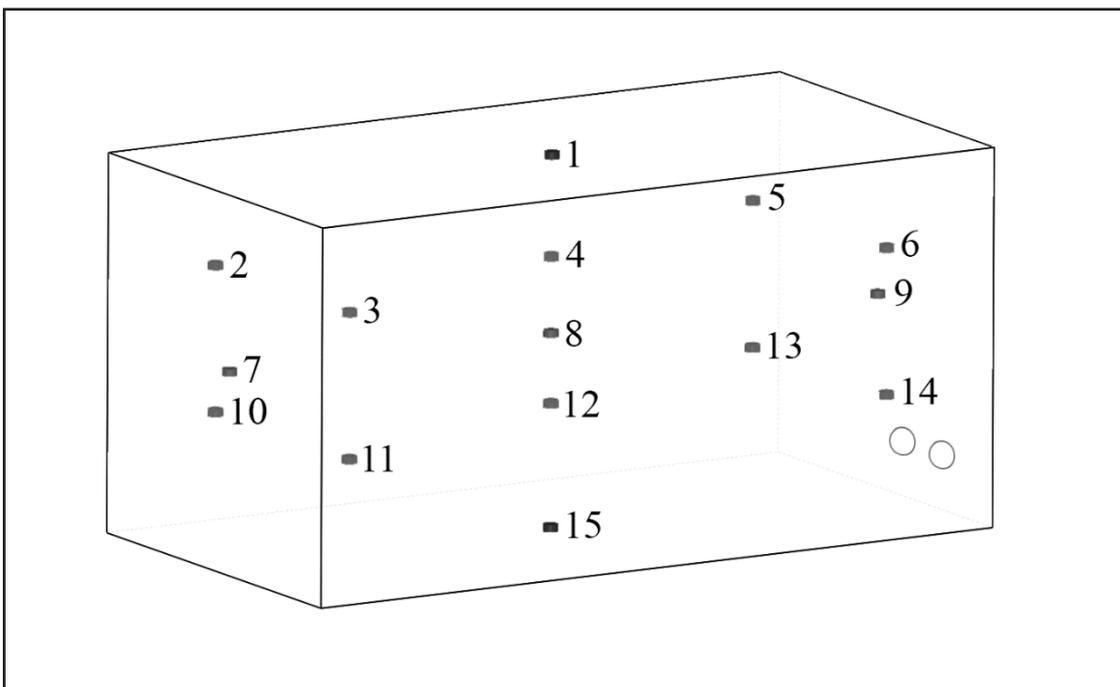
According to (ANDRADE *et al.*, 2004), the error found for the temperature distribution for the simulation of storage in a natural environment is consistent with that found in the literature, with a mean estimated error of 2.6% for the simulation of corn storage in a metallic silo. (XI *et al.*, 2016) found a mean estimated error of approximately 4.0% for the simulation of wheat storage.

The literature on the simulation of the temperature distribution in the storage of agricultural products in a cooled environment is limited, and even fewer studies show the percentage errors obtained by the model. (HAN *et al.* 2019) simulated the cool storage of apples on a small scale and obtained a mean relative error for the temperature distribution of 4.9% for a simulation using the same turbulence model (standard k-ε). Akdemir and Bartzanas (2015) simulated the cooled storage of apples and obtained an error of 13% for the temperature distribution in the system.

The sensors were numbered from 1 to 15 to designate the individual results for each sensor in the coffee pile in a cooled environment, as shown in Figure 7.

The division of the sensors by height in the pile was as follows: top - 1; upper- 2, 3, 4, 5, and 6; middle - 7, 8, and 9; lower - 10, 11, 12, 13 and 14; and bottom - 15. Figure 8 shows the temperature obtained experimentally for each of the 15 collection points and obtained by the model throughout the cooled storage as well as the mean relative error.

Figure 7 – Number associated with each temperature sensor in the storage in a cooled environment



Source: Author (2020)

Figure 8 – Temperatures obtained experimentally and by the model during cooled storage and mean relative error (P) for each collection point

(Continued)

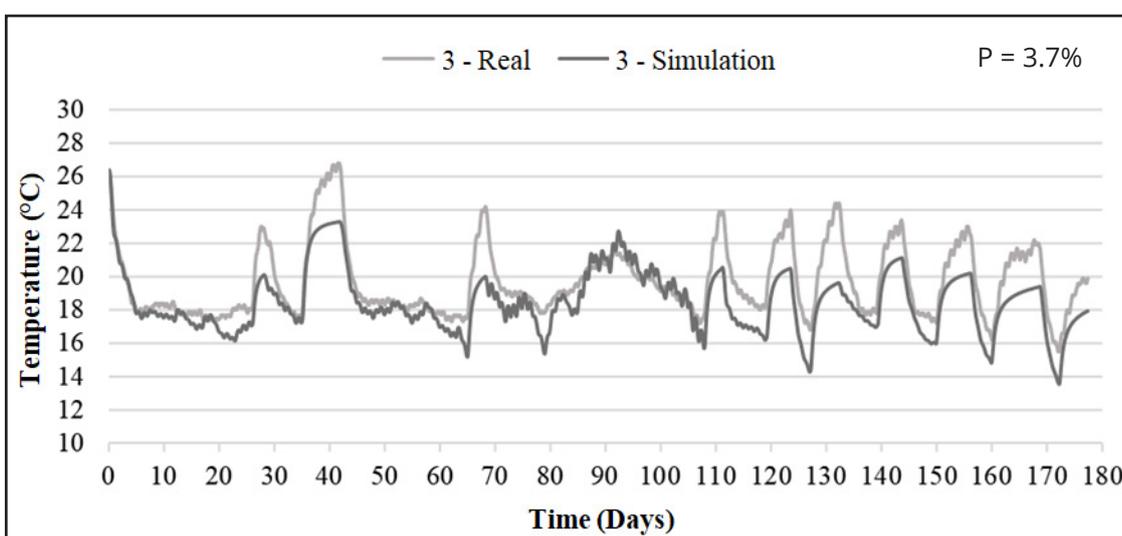
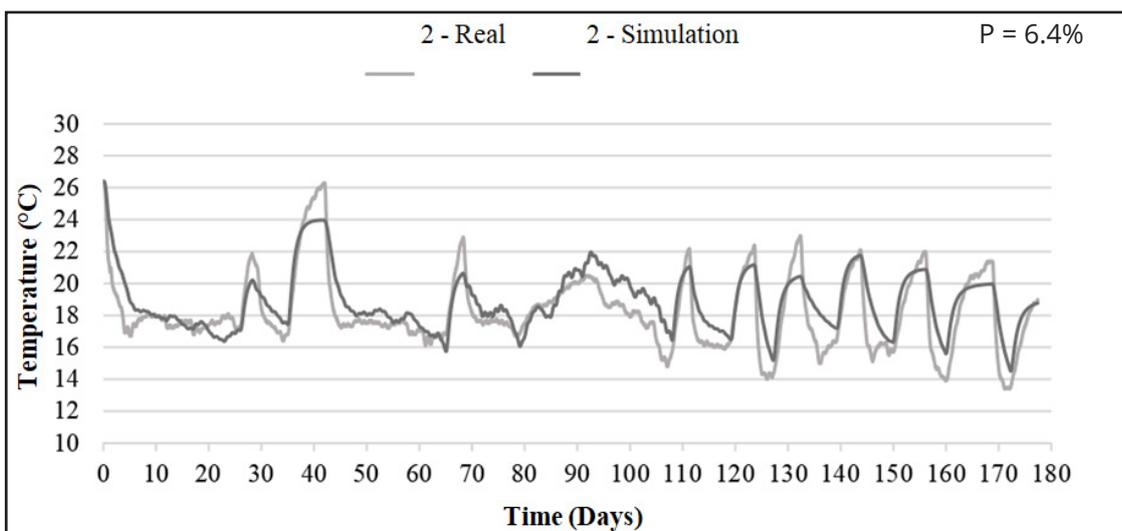
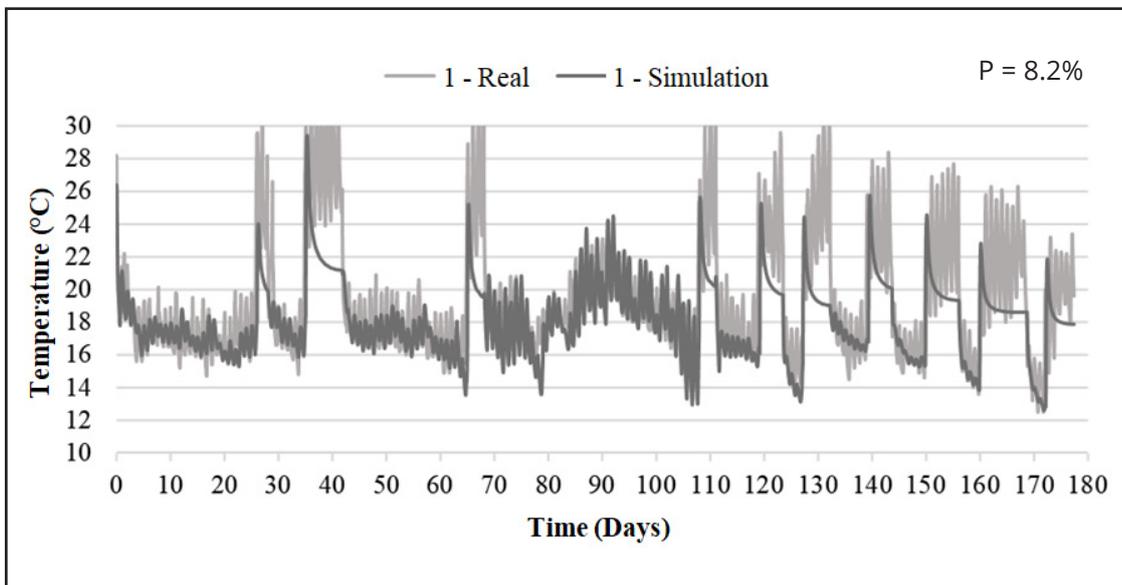


Figure 8 – Temperatures obtained experimentally and by the model during cooled storage and mean relative error (P) for each collection point

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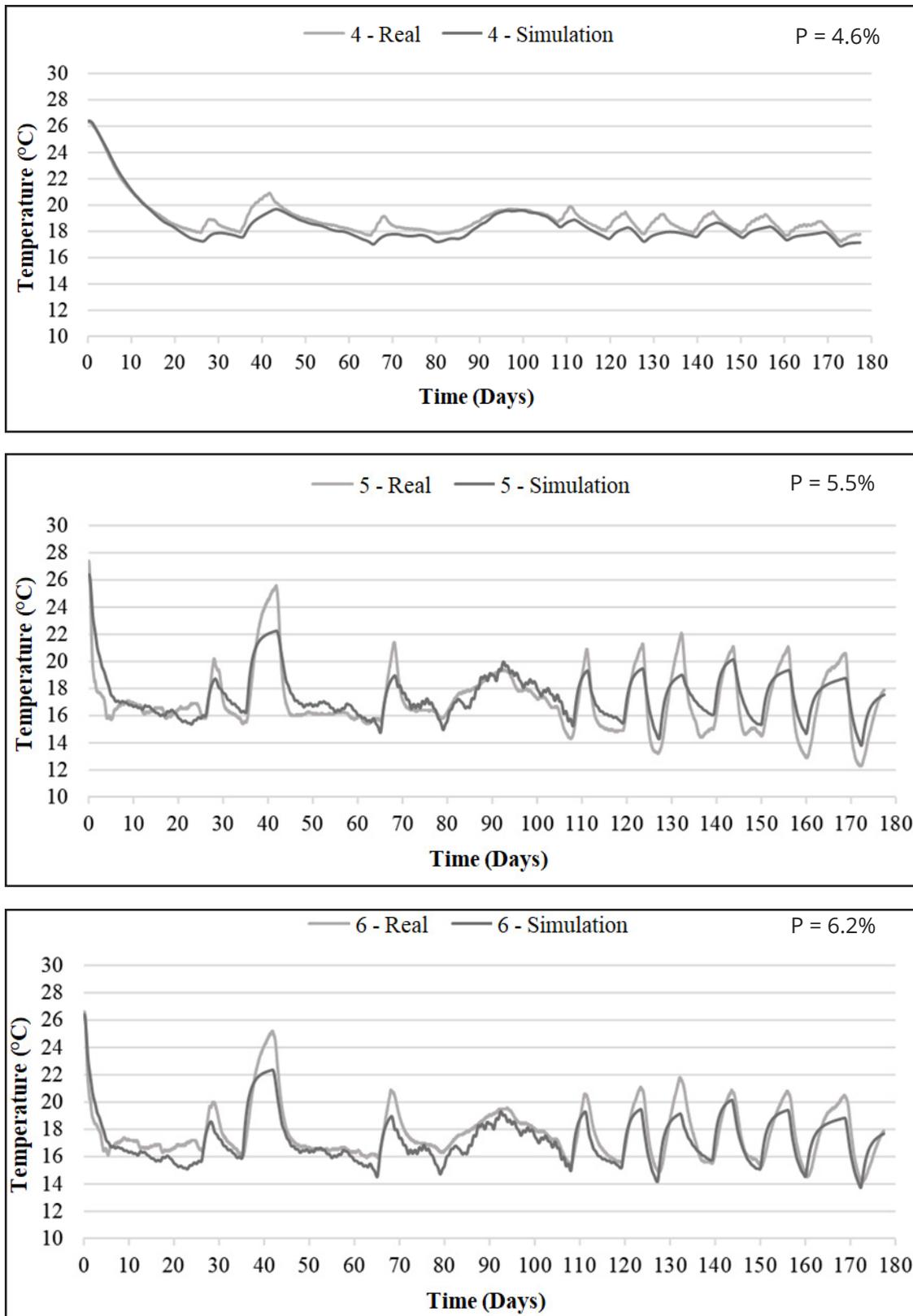


Figure 8 - Temperatures obtained experimentally and by the model during cooled storage and mean relative error (P) for each collection point (Continued)

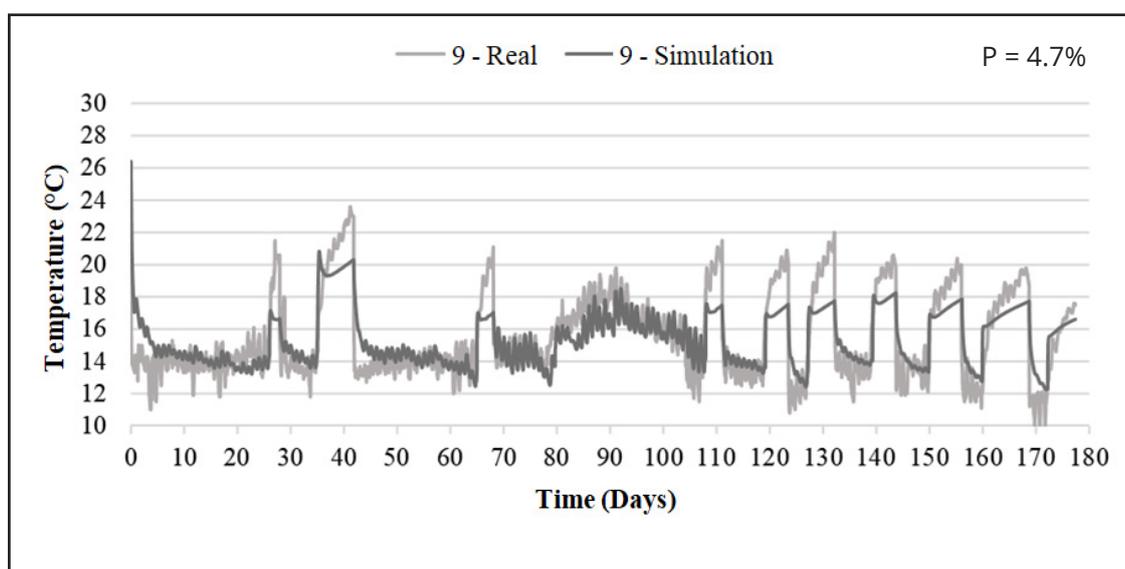
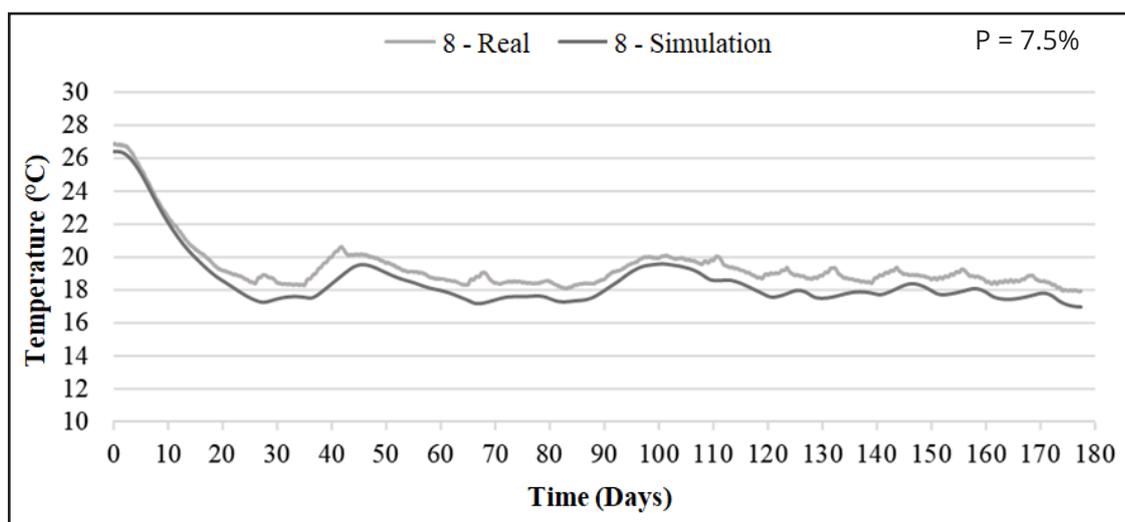
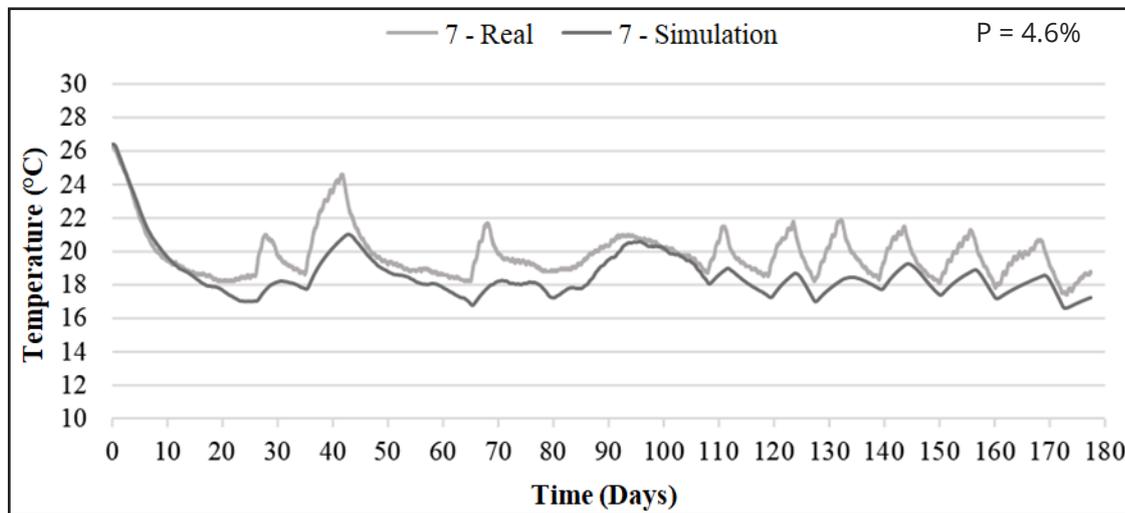


Figure 8 - Temperatures obtained experimentally and by the model during cooled storage and mean relative error (P) for each collection point

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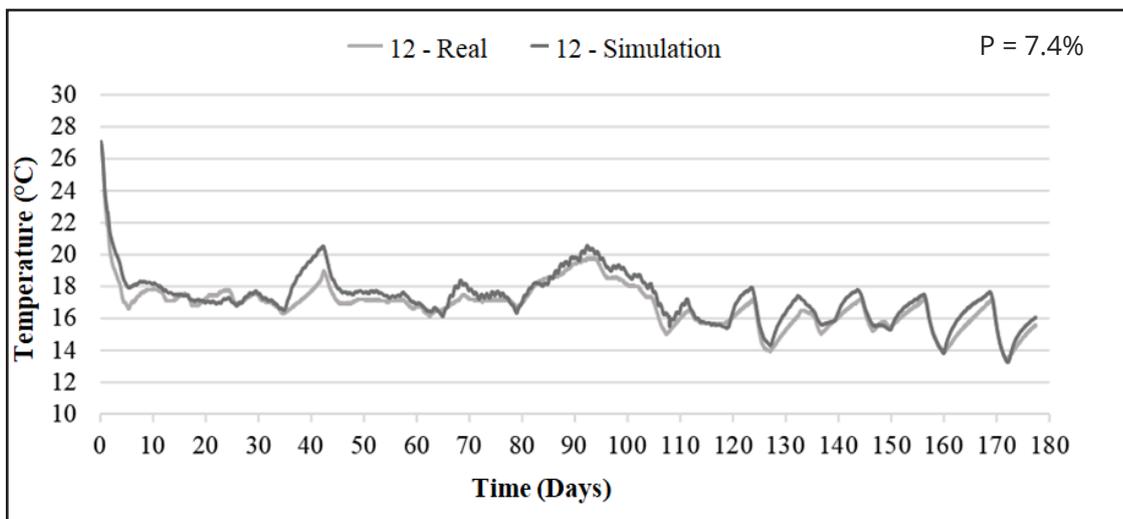
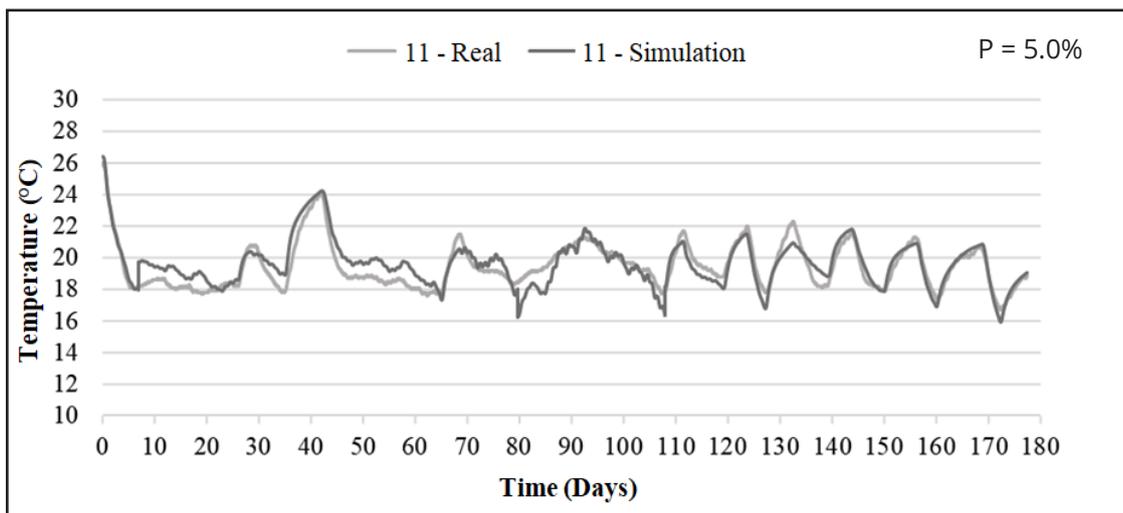
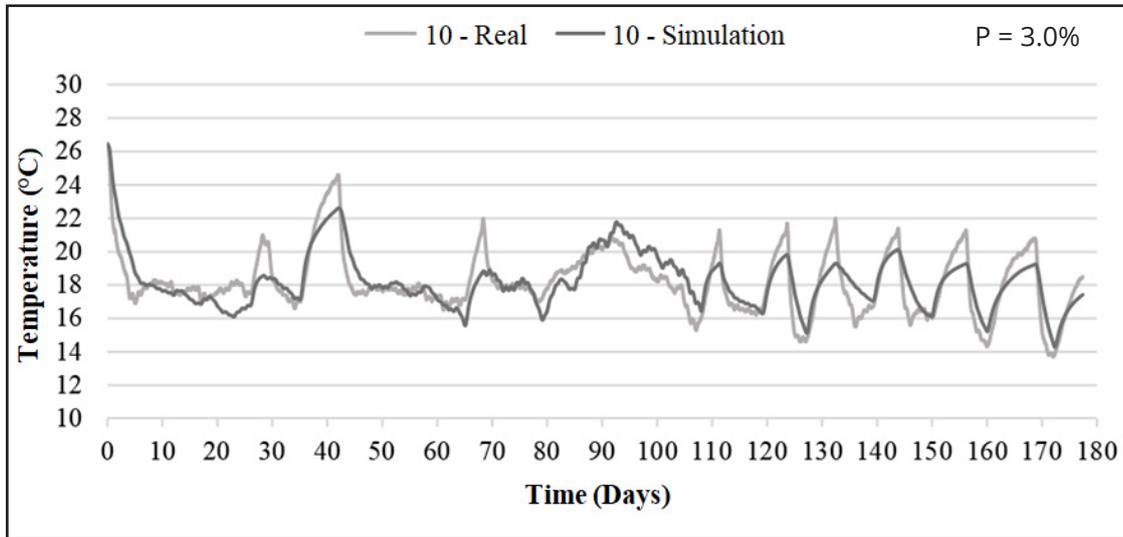
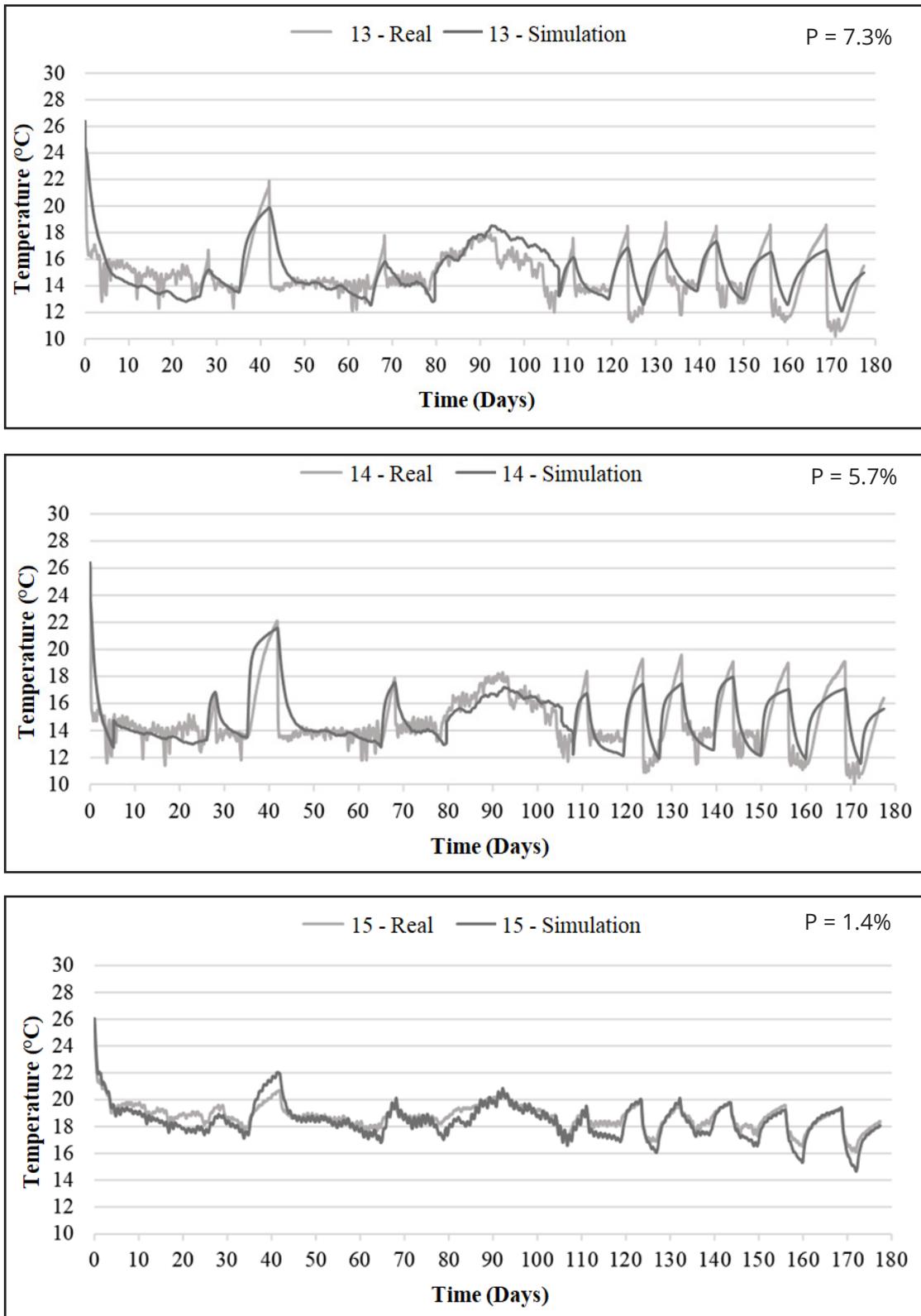


Figure 8 – Temperatures obtained experimentally and by the model during cooled storage and mean relative error (P) for each collection point

(Conclusion)

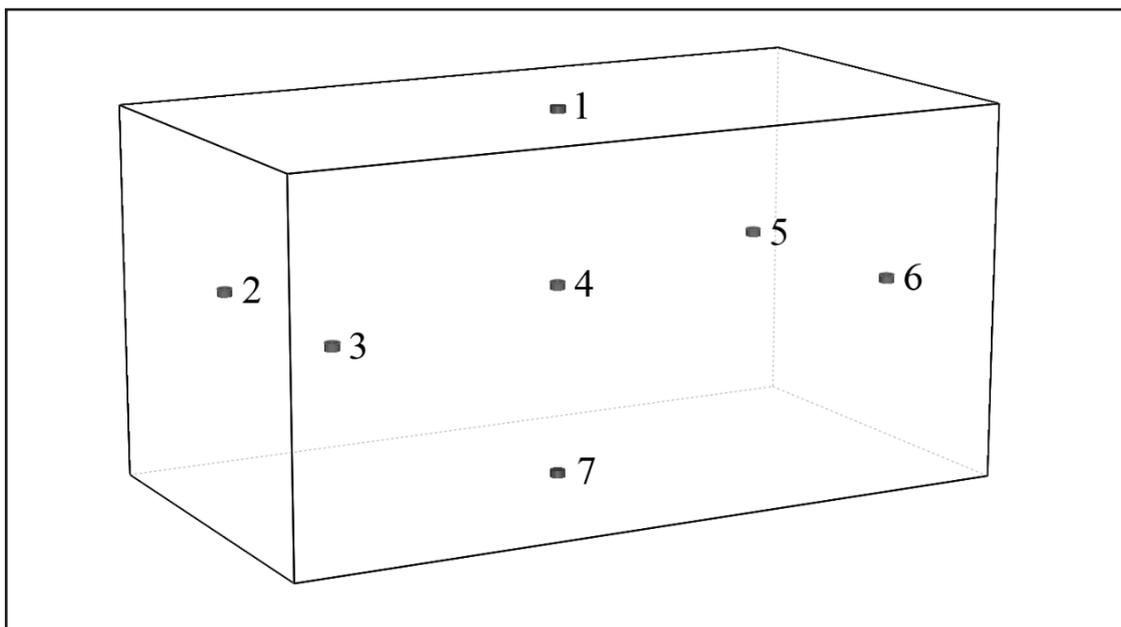


Source: Author (2020)

The points with the highest mean relative error were "1" (8.2%), "9" (7.5%), "13" (7.4%) and "14" (7.3%). These higher values can be explained as follows: point "1" was the sensor at the top of the pile and was the most exposed to changes in external temperature and cooled air circulating in the system; points "9", "13" and "14" were the closest to the cooled air inlets and were more susceptible to rapid changes in temperature caused by turning the refrigeration equipment on and off. The other points had a mean relative error between 3.0 and 6.5%.

For the presentation of the individual result for each sensor in the coffee pile in a natural environment, the sensors were numbered from 1 to 7, as shown in Figure 9.

Figure 9 – Number associated with each temperature sensor in the natural environment storage



Source: Author (2020)

It is important to note that sensor "1" was above the coffee pile during the entire storage time, recording the local ambient temperature data. These data were used as boundary conditions for both storage systems. Therefore, this collection point was not simulated or compared and was not included in the determination of the overall mean relative error previously presented.

Figure 10 shows the temperature obtained experimentally and by the model throughout natural storage and the mean relative error for each sensor in the coffee pile

Figure 10 – Temperatures obtained experimentally and by the model during natural storage and mean relative error (P) for each collection point

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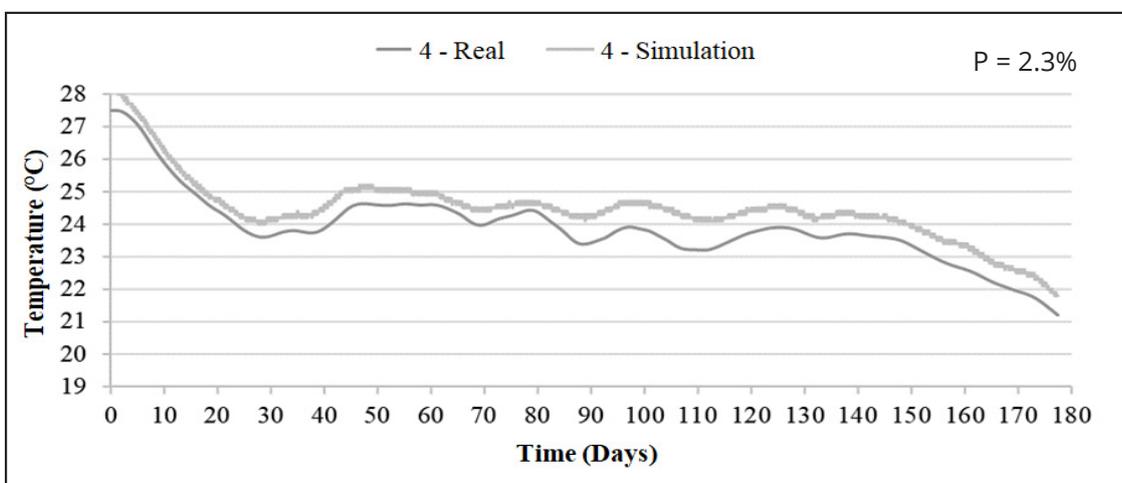
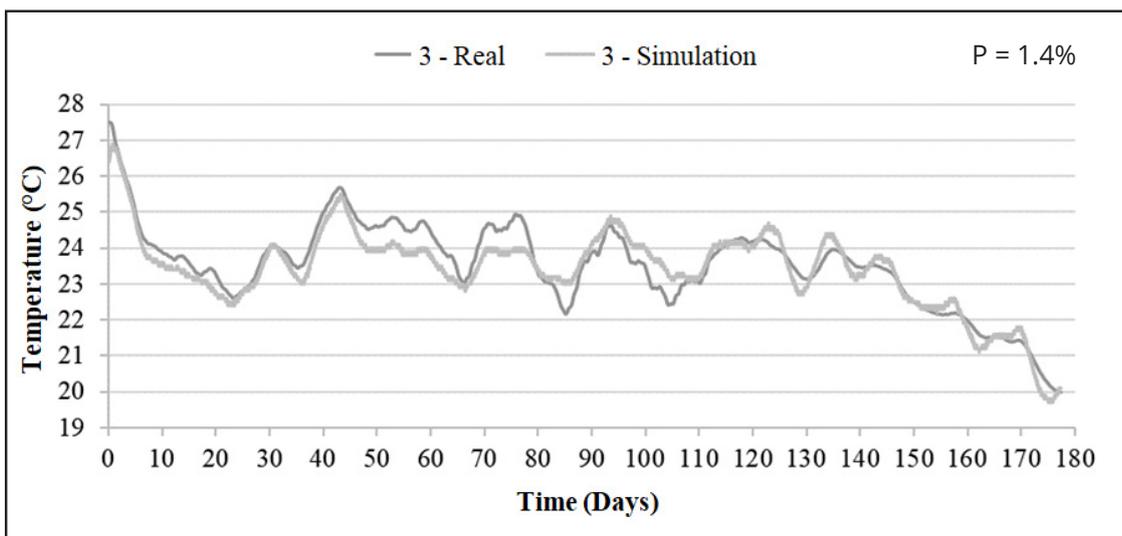
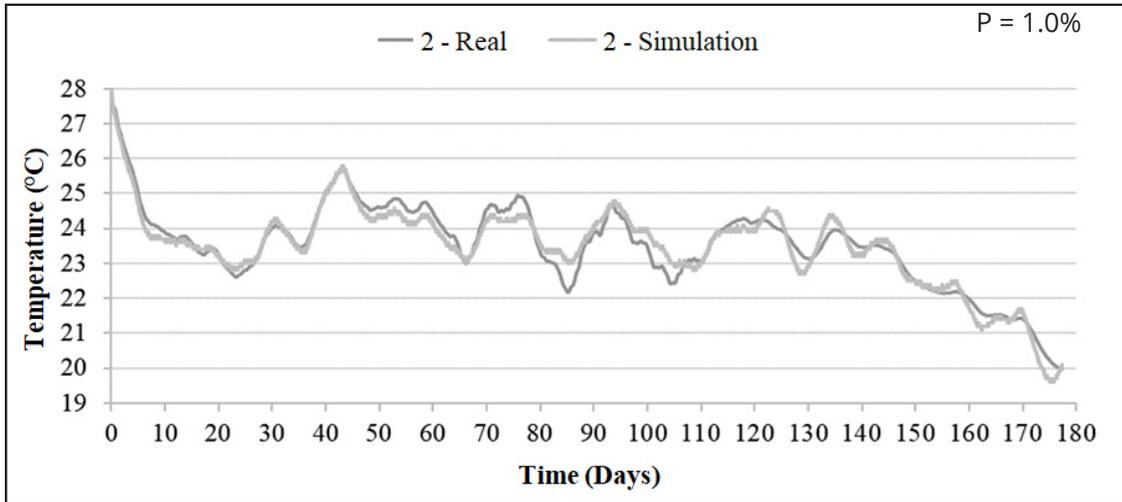
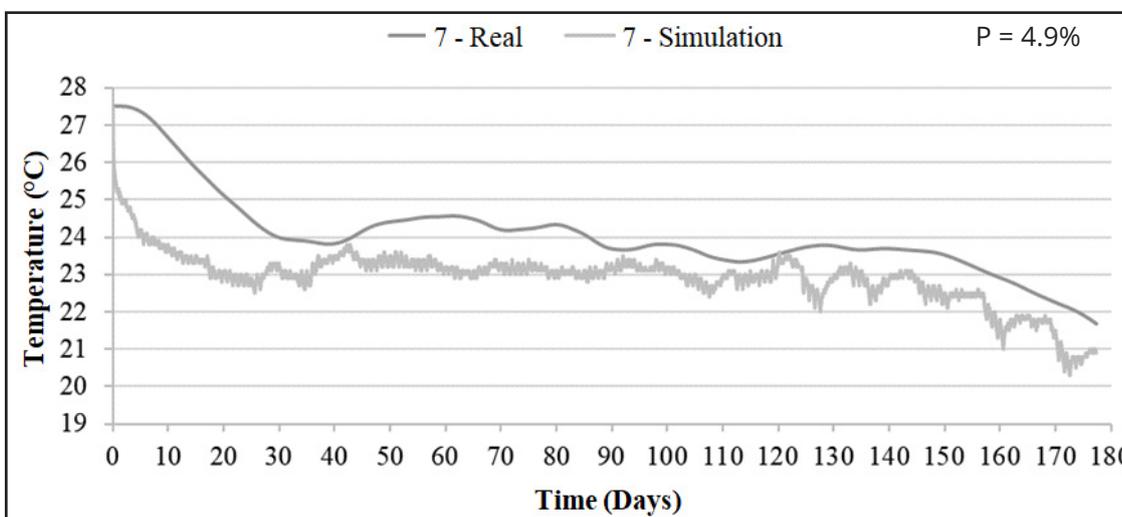
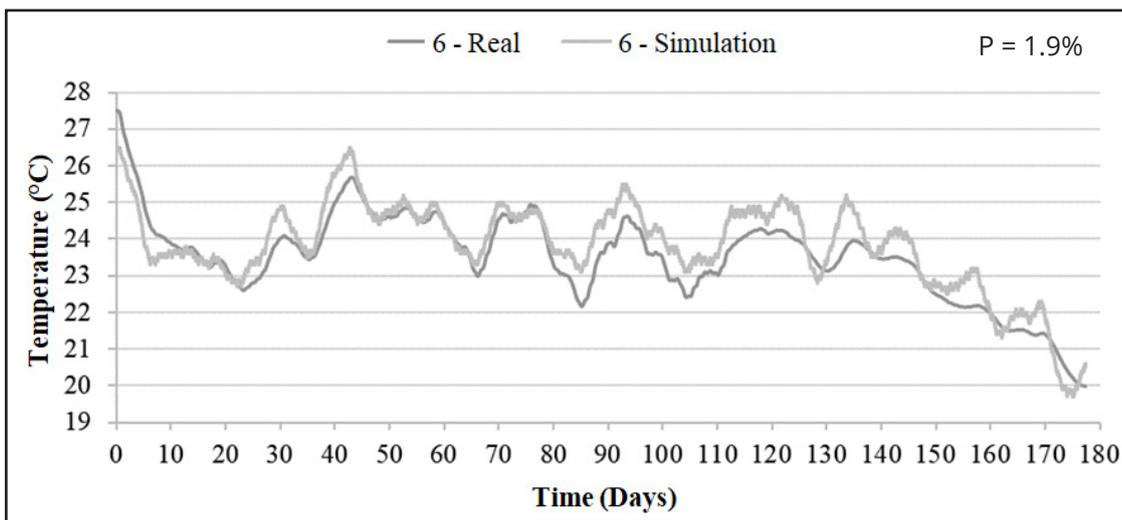
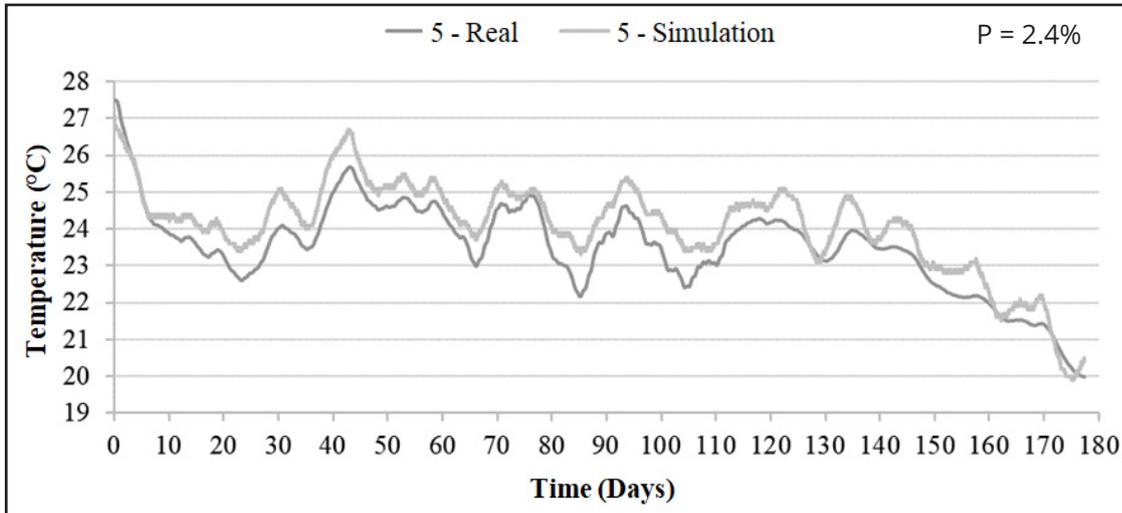


Figure 10 – Temperatures obtained experimentally and by the model during natural storage and mean relative error (P) for each collection point (Conclusion)

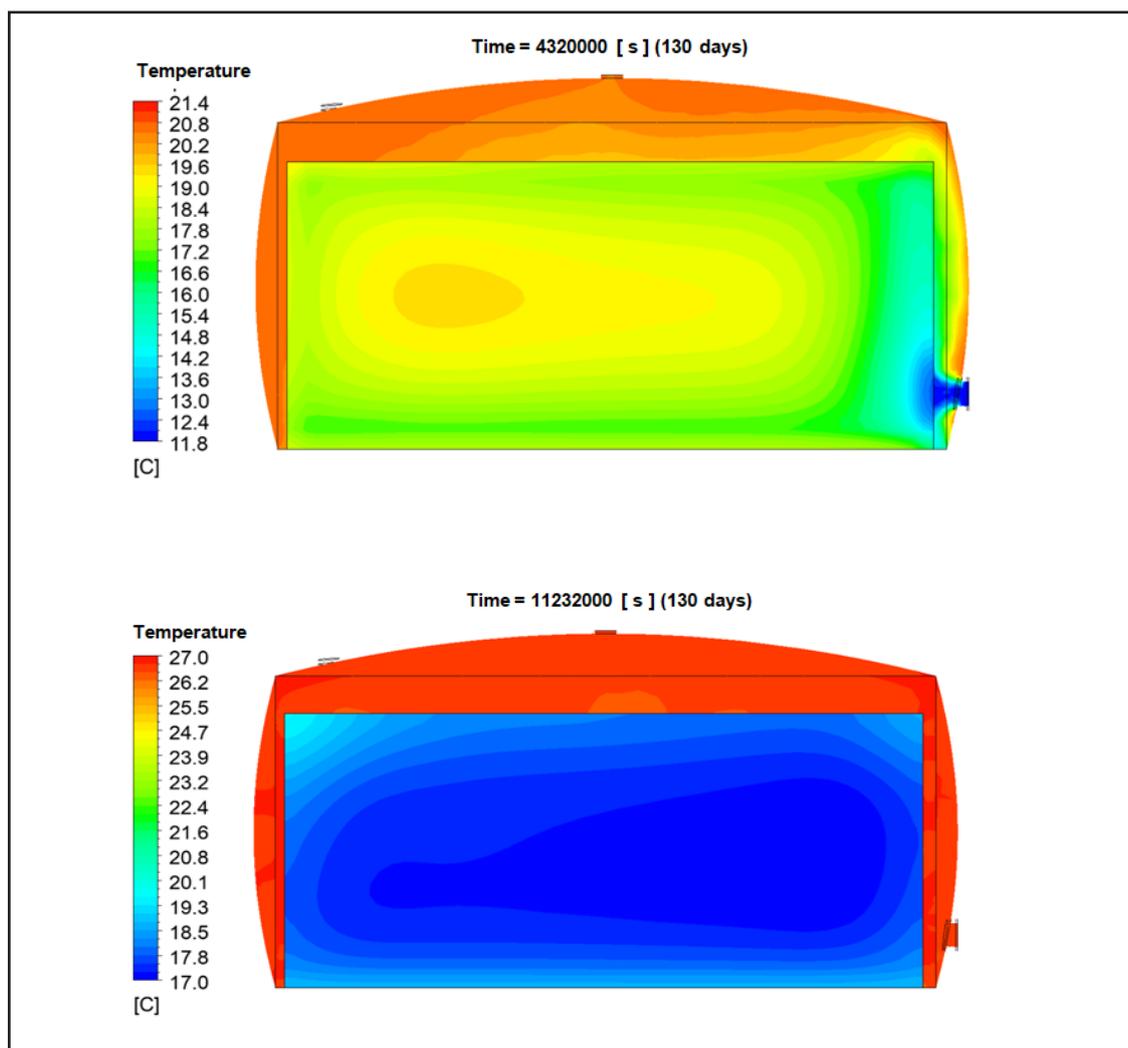


Source: Author (2020)

Point “7” showed a higher relative error (4.9%), which can be explained by its greater proximity to the outside of the coffee pile. The other points had mean relative errors between 1.0 and 2.5%.

Figure 11 below shows examples of the temperature distribution through a vertical section in the center of the system for storage in a cooled environment. The times shown are 4,320,000 seconds (50 days), during the period in which the cooling system was turned on and cool air was introduced into the cocoon, and 11,232,000 seconds (130 days), during the period when the cooling system was turned off.

Figure 11 – Distribution of the internal temperature of the coffee pile and cocoon at 50 days (A) and 130 days (B) after storage in a cooled environment

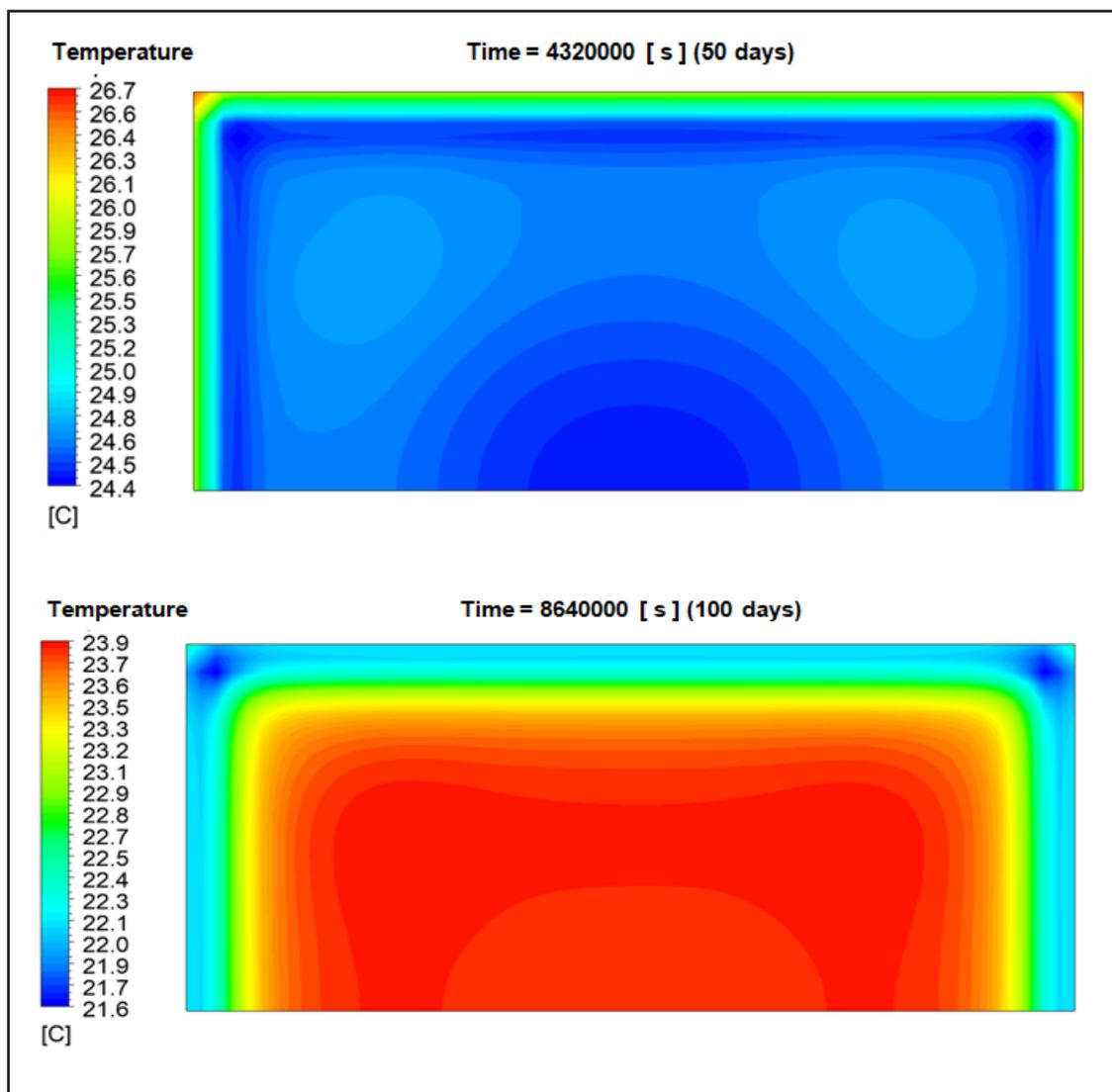


Source: Author(2020)

It is possible to note differences in the temperatures inside the coffee pile and in the air around it when the system was being cooled and when it was not.

Similarly, Figure 12 below shows the temperature distribution obtained by the model at times of 4,320,000 seconds (50 days) and 8,640,000 seconds (100 days) through a vertical cut in the center of the system for storage in a natural environment. In this case, it is possible to see the temperature differences inside the coffee pile, which remains in contact with the external environment at all times.

Figure 12 – Vertical section of the internal temperature distribution in the coffee pile at 50days (A) and 100 days (B) after storage in a natural environment



Source: Author (2020)

Note that the external temperature at 4,320,000 seconds was higher than that in the inside of the coffee pile, which caused the outer stacks of coffee to warm up; in turn, the external temperature at 8,640,000 seconds was lower than that in the inner stacks, which cooled the outermost stacks. This occurred because the pile was always directly exposed to the environment, making the outermost stacks much more susceptible to external temperature changes.

4 CONCLUSIONS

Mocha coffee was stored for 6 months in two storage systems: a cooled environment and a natural environment.

The experimental results obtained in the cooled environment showed that the system used for storage in the cooled environment was unable to maintain the temperature within the desired limit (15 – 18 °C) and that the mean temperature was maintained between approximately 15 and 21 °C. Thus, the system used is not suitable for storage in a cooled environment, but note that the product used for the cocoon is not intended for thermal insulation of the product stored in its interior and was used in this study as a physical wrap to limit the passage of cooled air through the pile of grain bags; for this reason, an unsatisfactory performance was obtained. Possible alternatives for improving the overall efficiency of the system include the use of a wrap specifically for thermal insulation and the reuse of the cooled air leaving the cocoon so that it returns and is cooled and blown inside again; this would even improve the energy efficiency of the equipment.

The computational models used to simulate the operation of each storage system showed mean relative errors of less than 10%, which indicates that numerical simulation (using the joint CFD–FEM approach) can be used to predict the temperature distribution behavior in stored coffee piles both in a natural environment and in an environment with cooled air injection. This implies that the actual conditions can be represented by the model with an acceptable error and that any alternatives tested

in the system could be tested directly in the computational model, which would give a good representation of how the new conditions would perform and allow greater efficiency and reduced costs in the experimentation process.

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